

# Application of Hypervirial Theorem As Criteria For Accuracy of Variational Trial Wave Function

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## Abstract

It would be interesting to investigate the accuracy of the results obtained in the variational method, because it is important for studying hadron spectra. One can define some criteria to judge the accuracy, or the quality of the trial function. We employ a simple potential form to check how accurate the variational results obtained by a single-parameter trial function can be. All the concerned problems, in particular, the relevant aspects on the application of hypervirial theorem in variational method for various potential forms, are discussed in every detail. The qualitative conclusion of the work can be generalized to much more complicated cases. Our study suggests that the hypervirial relations can serve as a good and practical criterion for judging the accuracy of any trial functions.

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## I. INTRODUCTION

As well known, there are few potential forms whose bound state problems can analytically be solved. Therefore, various approximate methods have been used to do the job, in which, no doubt, numerically solving the Schrödinger equation is the most direct and powerful method, which in principle can meet any desired accuracy. But on other side, it cannot provide analytical expressions for further discussions. Moreover, usually, as one numerically solves the Schrödinger equation, he can only keep a few terms in the zero-th order, while leaving the others, such as the spin-dependent terms to be treated as a perturbation. Indeed, the perturbative method is an approximate treatment which has extensively been adopted because of its simplicity and convenience. However, this method is limited by the convergence of perturbative expansion. In fact, treating wave functions is much more difficult than evaluating energy eigenvalues [1].

Another widely employed approach is the variational method. Most desirable advantage of the method is that there exists an analytical expression of the wave function for further discussions on physics. In past years, lots of work paid their attention to seeking for accurate energy eigenvalues but seldom discussed the wave function. In many simple cases, the Gaussian-type or the exponential-type trial wave functions (TWF) with a single variational parameter are employed and they usually can give an accurate value for the eigenenergy, but it is not true for the wave function in general.

In a recent work [2], we investigated this problem in detail with various potential forms which are used frequently in literatures to study heavy quarkonia and put more emphases on estimating the wave function at origin (WFO) by using a TWF with single and several variational parameters. We hope that it would shed some light on how to obtain sufficiently accurate WFO in terms of the variational method. We find that the accuracy of WFO seriously depends on the choice of the forms of TWF. In general, although there is no universal rule to determine the form and the number of the parameters of the TWF, one can always find out a relatively simple and more reliable TWF with the least number of parameters. Our result showed an economic way to realize it.

Recently, Lucha and Schöberl have made a renewed investigation [3] to qualitatively and quantitatively evaluate the accuracy, namely how close to the exact eigenstates the results obtained in variational method can be. They embark upon a systematic study of the accuracy of the variationally determined eigenstates of a Hamiltonian  $H$  and suitable measures to judge their quality and apply their principles to the prototype of all (semi-) relativistic bound-state equations, the “spinless Salpeter equation”. In their work, the harmonic-oscillator potential is employed as an example. Their work is very instructive and stimulates interest in studying the accuracy of the trial wave function for the variational method. It is the goal of this work to further study the accuracy of the TWF with single variational parameter and the criteria to judge the accuracy.

In this work, we firstly extend the criteria used by the authors of Ref. [3] and apply them to treat a simple case of the non-relativistic Schrödinger equation where only the linear potential exists and give some further discussions on the accuracy of the TWF with single parameter. The motivation to choose the linear potential is three-fold. The first is its significance in the particle physics. The next is that if only the linear potential exists, there are exact solutions for  $nS$  states, which are the well-known Airy function  $\text{Ai}(z)$ . Thus,

we can conveniently use them as a basis for comparing the results obtained with the TWF and the exact one to quantify how close to each other the approximate solutions in the variational method and exact eigenstates can be. The last one is that we find that the linear potential possesses some interesting features which are helpful for a thorough investigation of the criteria which can be generalized to other cases.

After the quantitative discussion to all the criteria for the ground states and the lowest radial excitation state of the linear potential, we study in detail the application of hypervirial relations as a most powerful and practical criterion to judge the accuracy of the variational trial wave function. We shall prove that when the variational parameter  $a$  take its optimal value, the special form of the TWF

$$R_{twf}^{(n)}(r) = N_n r^n e^{-a r^b}$$

satisfies the general virial theorem which is so called the first order hypervirial relation. This is independent of both the concrete form of the central potential and the specific value of  $b$ . In this case we have to use higher order hypervirial relations as a criterion to judge the quality of the TWF. To further testify the applications of the hypervirial theorem, we calculate the relevant quantities corresponding to several commonly adopted potential forms such as the Cornell, logarithmic, Martin's and power-like ones.

The paper is organized as following. After the introduction, we provide several criteria for judging the quality of the TWF, where the linear potential is taken as an example to serve as the basis for discussion. Indeed applications of all of them need to priori know the exact solutions for a comparison, studying them is to find support to our main goal, i.e. to apply the hypervirial relations as criteria. In Sec.III, we discuss applications of the hypervirial relations which can serve as practical and useful criteria for the quality of the TWF. In the last section, discussion and conclusion are made.

## II. SEVERAL EXACT-SOLUTION-DEPENDENT CRITERIA FOR TWF

What we concern is how close to the accurate solution the obtained approximate wave function can be when the approximate energy  $E_{min}$  of Eq.(B5 in the Appendix B) is satisfactorily close to the accurate energy eigenvalue, or in other words, how seriously the approximate  $R_{twf}$  deviate from the real one and how the nature and extent of these errors affect the calculated values. There were intensive discussions on the problem many years ago [4]. Recently Lucha and Schöberl [3] reviewed and developed these discussions and introduced several measures to judge the quality of an approximate wave function in the variational method, whose applications to our case are described in the following.

(a) The distance between the obtained approximate value of the energy  $E_{min}$  and exact eigenvalue  $E$ . It can be represented by using the relative error  $\varepsilon$  of  $E_{min}$  and  $E$ ,

$$\varepsilon \equiv \frac{E_{min} - E}{E} . \quad (1)$$

(b) The overlap integral  $S$  of the trial state  $|R_{twf}\rangle$  and the eigenstate  $|R_{eig}\rangle$ .

If both  $|R_{twf}\rangle$  and  $|R_{eig}\rangle$  are normalized, i.e.

$$\langle R_{twf}|R_{twf}\rangle = \langle R_{eig}|R_{eig}\rangle = 1,$$

one can define

$$S = \langle R_{twf}|R_{eig}\rangle. \quad (2)$$

If the  $R_{twf}$  is just the exact eigen-state  $R_{eig}$ , the overlap  $S$  is equal to unity. In general, we have

$$0 \leq |S| \leq 1.$$

As a quantitative criterion, according to the suggestion of authors of [3], we take the deviation of the squared modules of the overlap  $S$ , from unity,  $\sigma$  as

$$\sigma \equiv 1 - |S|^2. \quad (3)$$

(c) The normalized maximum difference of variational function  $R_{twf}(r)$  and the eigenstate  $R_{eig}(r)$ , i.e., the maximum relative error,

$$\omega \equiv \frac{\max_{\mathbf{r}} [R_{twf}(r) - R_{eig}(r)]}{\max_{\mathbf{r}} R_{eig}(r)}. \quad (4)$$

Besides the above criteria, we introduce the following measures which may reveal the physical properties of the TWF.

(d) The squared wave function at origin (WFO)  $R^2(0)$ .

As is noticed in our earlier work [2], this quantity can be obtained by using two methods. The first approximate WFO,  $R^2(0)$  **I**, is directly calculated from the normalized radial wave function by setting  $r = 0$ . And in the second approach,  $R(0)^2$  **II** can be obtained from the well-known equation [5]

$$R^2(0) = 2\mu \langle R | \frac{dV}{dr} | R \rangle. \quad (5)$$

If  $R(r)$  is the real solution of the Schrödinger equation with the given potential, the resultant  $R(0)^2$  **I** and  $R(0)^2$  **II** should exactly be the same. However, if we use  $R_{twf}(r)$  to calculate these two quantities, the results definitely deviate from each other. Our numerical results [2] showed that the later one can generally reach very high accuracy.

In the present case of the linear potential  $V(r) = r$  with  $2\mu = 1GeV$ , it is very easy to prove that the resultant  $R(0)^2$  **II** is

$$R^2(0) = \langle R | R \rangle. \quad (6)$$

Thus, for the any  $R(r)$ , no matter it is an accurate eigen-wavefunction  $R_{eig}(r)$  or any TWF  $R_{twf}(r)$ , so long as it satisfies the normalization condition, the  $R(0)^2$  obtained by using such method must be identical to unity. Definitely, this is a special feature possessed by the  $S$ -wave bound state for the linear potential. Therefore, we only have the first type of the WFO  $R(0)^2$  **I** can be used in our case. In practice, what we take as a quantitative criterion is the relative deviation

$$\delta r_{02} \equiv \frac{R_{twf}^2(0) - R_{eig}^2(0)}{R_{eig}^2(0)}. \quad (7)$$

However, in the general case,  $dV/dr \neq 1$ , then both  $R^2(0)\mathbf{I}$  and  $R^2(0)\mathbf{II}$  can be used to obtain  $\delta r_{02}$ .

(e) The average value of the operators  $r^2$  and  $r^{-2}$ .

In order to show the effect of the approximate wave function on some particular properties, we calculate average values  $\langle r^2 \rangle$  and  $\langle r^{-2} \rangle$ . In fact, the weighted overlap integrals [4] depend principally on regions of the configuration space. The accuracy of  $\langle r^2 \rangle$  depends mainly on the accuracy of TWF in the outer regions and that of  $\langle r^{-2} \rangle$  depends more sensitively on the region near the origin. In practice, what we select as the criteria are the relative errors of the approximate value with respect to the exact one

$$\delta r_{p2} \equiv \frac{\langle R_{twf} | r^2 | R_{twf} \rangle - \langle R_{eig} | r^2 | R_{eig} \rangle}{\langle R_{eig} | r^2 | R_{eig} \rangle} \quad (8)$$

and

$$\delta r_{n2} \equiv \frac{\langle R_{twf} | r^{-2} | R_{twf} \rangle - \langle R_{eig} | r^{-2} | R_{eig} \rangle}{\langle R_{eig} | r^{-2} | R_{eig} \rangle}. \quad (9)$$

All the numerical results corresponding to these criteria for the ground state and low excitations of the linear potential, including the values of the optimal variational parameter  $a_0$ , the minimum values of the energy  $E_{min}$ , are listed in Table 1.

The numerical results in Table 1 confirm that all the criteria can be effectively used for judging the quality of the TWF.

### III. THE HYPERVIRIAL RELATIONS AS MOST PRACTICAL AND POWERFUL CRITERIA

#### A. The hypervirial theorem and hypervirial relations

The virial theorem has been widely used in both classical and quantum mechanics. In quantum mechanics, it can be formulated as

$$2 \langle T \rangle = \langle \vec{r} \cdot \nabla V(r) \rangle,$$

where  $T$  is the kinetic energy operator and the expectation value is taken for eigenwavefunctions of the Hamiltonian  $H$ . It holds for any central potential  $V(r)$ .

It is easy to prove that an equivalent statement of the virial theorem is that the expectation value of the commutator  $[W, H]$  on the energy eigenstates  $|R_{eig}\rangle$ , vanishes:

$$\langle R_{eig} | [W, H] | R_{eig} \rangle = 0. \quad (10)$$

where

$$W = \frac{1}{2}(\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}), \quad (11)$$

is called as the generator of dilatations and  $H$  is the Hamiltonian.

Hirschfelder generalized the theorem to the so called hypervirial theorem [6]. It states that the expectation value of the commutator  $[G, H]$ , where  $G$  stands for any time-independent linear operator, on the energy eigenstate  $|R_{eig}\rangle$  is equal to zero:

$$\langle R_{eig} | [G, H] | R_{eig} \rangle = 0. \quad (12)$$

Obviously our  $W$  is such an operator.

However, for a trial state  $|R_{twf}\rangle$ , in general, the expectation value  $\langle R_{twf} | [G, H] | R_{twf} \rangle$  is not equal to zero. We can expect that the closer to the real solution the approximate trial function is, the closer to zero the expectation value would be. Hence, a set of operators  $G$  generates a whole set of the "hypervirial relations", which will be defined in Eq.(19), and each of them may serve as a measure of the quality of a given trial function  $|R_{twf}\rangle$  by evaluating the expectation value  $\langle R_{twf} | [G, H] | R_{twf} \rangle$ .

In the present work, the hypervirial operator can be chosen as [7,8]

$$G = f(r)p_r \quad (13)$$

where  $f(r)$  is a function of  $r$  and  $p_r$  is the radial momentum operator conjugate to  $r$ , whose explicit expression is  $p_r = -i(d/dr + 1/r)$ . The corresponding Hamiltonian (with  $2\mu = 1$  GeV) reads

$$H = (p_r)^2 + \frac{l(l+1)}{r^2} + V(r). \quad (14)$$

Considering

$$\begin{aligned} [G, H] &\equiv [f(r)p_r, H] \\ &= 2i\frac{df(r)}{dr}p_r^2 + i\frac{d^2f(r)}{dr^2}p_r + 2if(r)\frac{l(l+1)}{r^3} - if(r)\frac{dV}{dr}, \end{aligned} \quad (15)$$

$$p_r^2 = H - \frac{l(l+1)}{r^2} - V \quad (16)$$

and

$$\frac{d^2f(r)}{dr^2}p_r = \frac{i}{2}\frac{d^3f(r)}{dr^3} - [\frac{df(r)}{dr}, H], \quad (17)$$

we can get the commutator

$$\begin{aligned} [G, H] &= 2i\frac{df(r)}{dr}(H - V) + 2il(l+1)(\frac{f(r)}{r^3} - \frac{1}{r^2}\frac{df(r)}{dr}) + \frac{i}{2}\frac{d^3f(r)}{dr^3} \\ &\quad - if(r)\frac{dV}{dr} - \frac{i}{2}[\frac{df(r)}{dr}, H]. \end{aligned} \quad (18)$$

The hypervirial theorem demands the expectation values of both  $[G, H]$  and  $[\frac{df(r)}{dr}, H]$  for the eigenstate of  $H$  to be zero, thus from Eq. (18) we can obtain an algebraic equation

$$2E\langle\frac{df(r)}{dr}\rangle = 2\langle V\frac{df(r)}{dr}\rangle + \langle f(r)\frac{dV}{dr}\rangle - 2l(l+1)\langle\frac{f(r)}{r^3}\rangle - \langle\frac{1}{r^2}\frac{df(r)}{dr}\rangle - \frac{i}{2}\langle\frac{d^3}{dr^3}f(r)\rangle. \quad (19)$$

where  $\langle\cdots\rangle$  stands for the expectation value over the eigenstate. These algebraic equations (19) are defined as the hypervirial relations.

Taking

$$f(r) = r^N \quad (N = 1, 2, 3, \cdots),$$

Eqs. (18) and (19) can respectively be re-formed as

$$\begin{aligned} [G_N, H] &\equiv [r^N p_r, H] \\ &= 2iNr^{N-1}(H - V) - ir^N\frac{dV}{dr} - 2il(l+1)(N-1)r^{N-3} + \frac{i}{2}N(N-1)(N-2)r^{N-3} \\ &\quad - \frac{i}{2}[Nr^{N-1}, H] \end{aligned} \quad (20)$$

and

$$\begin{aligned} 2EN\langle r^{N-1}\rangle &= 2N\langle r^{N-1}V\rangle + \langle r^N(DV)\rangle + 2l(l+1)(N-1)\langle r^{N-3}\rangle \\ &\quad - \frac{1}{2}N(N-1)(N-2)\langle r^{N-3}\rangle, \end{aligned} \quad (21)$$

where  $G_N = r^N p_r$  is the adopted hypervirial operators and Eq.(21) is an important recurrence relation which has extensive applications.

For the  $nS$  state in the linear potential case, we can obtain, from Eq.(19), a set of very useful recurrence relations

$$2EN\langle r^{N-1}\rangle = (2N+1)\langle r^N\rangle - \frac{1}{2}N(N-1)(N-2)\langle r^{N-3}\rangle, \quad (22)$$

which can be named the  $N$ -th order hypervirial relation.

When  $N = 1$ , we have the first order hypervirial relation

$$2E = 3\langle r\rangle, \quad (23)$$

which is just the general virial theorem in the linear potential case. Taking  $N = 2$  and  $N = 3$ , we can obtain the second and the third order hypervirial relation, which respectively are

$$4E\langle r\rangle = 5\langle r^2\rangle \quad (24)$$

and

$$6E\langle r\rangle = 7\langle r^3\rangle - 3. \quad (25)$$

In the above equations, the average is taken over the eigenstate of  $H$ .

## B. Deviation from the hypervirial relations as criteria for accuracy of TWF

As mentioned in the last subsection, for a properly chosen trial function  $R_{twf}(r)$ , these hypervirial relations should merely approximately hold. According to the 1-st, 2-nd and 3-rd hypervirial relations, we can respectively define deviations:

$$\nu_1 \equiv 2E - 3\langle r \rangle, \quad (26)$$

$$\nu_2 \equiv 4E\langle r \rangle - 5\langle r^2 \rangle, \quad (27)$$

and

$$\nu_3 \equiv -6E\langle r^2 \rangle + 7\langle r^3 \rangle - 3, \quad (28)$$

where the average value of  $r^N$  can be analytically calculated in terms of our TWF<sup>1</sup>. For the ground state, by using Eq. (B1) with the optimal variational parameter  $a_0$ , one has

$$\langle r^N \rangle = \frac{\Gamma(\frac{3+N}{b})}{\Gamma(\frac{3}{b})} \left( \frac{(1+b)\Gamma(\frac{1}{b})}{2\Gamma(\frac{4}{b})} \right)^{\frac{N}{3}}. \quad (29)$$

In terms of Eq.(29) and  $E_{min}$ , we can easily obtain the numerical values of  $\nu_1$ ,  $\nu_2$  and  $\nu_3$ . In order to evaluate hypervirial relations for judging the quality of TWF, we further introduce relative errors  $\delta\nu_i$  (i=1,2,3...) instead of  $\nu_i$  as

$$\delta\nu_1 \equiv \frac{|\nu_1|}{3\langle r \rangle}, \quad \delta\nu_2 \equiv \frac{|\nu_2|}{5\langle r^2 \rangle}, \quad \delta\nu_3 \equiv \frac{|\nu_3|}{7\langle r^3 \rangle}. \quad (30)$$

Obviously, these expressions (30) of  $\delta\nu_i$  are only valid for the linear potential, for other potential forms, the denominators in (30) should be replaced.

The results of  $\nu_1, \delta\nu_1, \nu_2, \delta\nu_2, \nu_3$  and  $\delta\nu_3$  are listed in Table 1, respectively. In the next section, we will give more discussions on the implications of these results.

In this work, we specially choose the most frequently used hypervirial operators  $G_N = r^N p_r$ . When  $N = 1$ ,  $G_1 = r p_r$  has a clearly physical meaning. Although it itself is not a Hermitian operator, it only differs from its symmetrized and Hermitian form  $W$  (see Eq.(11)) by a constant, i.e.,

$$W = G_1 - \frac{i}{2}. \quad (31)$$

As a consequence,

$$[W, H] = [G_1, H],$$

and one obtains the same first order hypervirial relation.

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<sup>1</sup>It is noted that in this subsection, the  $\langle \rangle$  stands for an average with respect to the trial wavefunction TWF



As well known [9], the dilation generator  $W$  generates the scaling transformation or dilation of the phase space, which is an important transformation not only to quantum mechanics but also to classical mechanics. Its classical equivalent  $\mathbf{r} \cdot \mathbf{p}$  has been used to derive a virial theorem in the classical mechanics.

Using the hypervirial relation of the quantum mechanics derived in terms of the operators  $G_N$ , one can derive many useful recurrence relations between  $\langle r^N \rangle$  and  $E$ . These relations can be used to gain approximate eigen-spectra and the expectation values of observables without solving the wave functions of bound states as well as to calculate the phase shifts and the amplitudes of the scattering processes more effectively than in the perturbative method. In this investigation, what we concern is another important application noticed by Lucha and Schöberl [3]. We will show that the hypervirial relations could be sensitive criteria for the accuracy of the solution by using the variational method. Of course, if we choose a more complicated form, we cannot have such compact expressions and the results of  $\nu_i$  and  $\delta\nu_i$  would be presented only numerically. Even so, the principle and the general conclusion hold.

In the last section, we give many criteria which can be used to judge the accuracy of TWF. It can be seen from Table 1 that all these criteria give a consistent result, by which we can select a most optimal TWF corresponding to  $b = \frac{7}{4}$  for 1S state of the linear potential from four possible value of  $b$ . However, the practical significance of these criteria to judge the accuracy of the TWF are limited by their dependence on the exact solution. It is clear that if one can get the exact solution, it, in general, would be unnecessary to find the approximate solution. But sometimes we want to use the variational method to find a simple analytical form of the approximate wave function with single parameter or a few parameters to replace a complicate exact solution or a pure numerical solution, and then these criteria are certainly very helpful. However, for those problems that we do not need an exact solution or it is very difficult to obtain the exact solution, these exact-solution-dependent quantities have no practical usage. In the case, as criteria the deviations from the hypervirial relations are the unique choice because only they do not require any knowledge on the exact eigen state and consequently can be applied to all the cases.

Table 1

The values of various criterion quantities for the single-parameter variational solutions of the 1S, 2S and 3S states in the linear potential case. The exact eigenvalues of energy are  $E_{1S} = 2.33810GeV$ ,  $E_{2S} = 4.08794GeV$  and  $E_{3S} = 5.52055GeV$ , respectively.

Quantity	1S state				2S state	3S state
b	1	$\frac{3}{2}$	$\frac{7}{4}$	2	$\frac{7}{4}$	$\frac{7}{4}$
$a_0$	0.908560	0.471405	0.348957	0.260531	0.348957	0.348957
$E_{min}$ (GeV)	2.47645	2.34723	2.33825	2.34478	4.09917	5.52874
$\varepsilon$	0.05917	0.00390	0.00006	0.00285	0.00275	0.00143
$\sigma$	0.032731	0.00207	0.00003	0.00180	0.00634	0.22584
$\omega$	0.14303	0.04353	-0.00436	0.35934	-0.0808	0.63515
$\delta r_{02}$	2.00000	0.33333	0.03646	-0.15117	-0.12956	-0.73780
$\delta r_{p2}$	0.24648	0.03070	-0.00086	-0.01264	-0.09030	-0.16022
$\delta r_{n2}$	0.46777	0.11295	-0.00790	-0.07351	0.01229	-0.30906
$\nu_1$	0	0	0	0	0.13701	0.23532
$\delta \nu_1$	0	0	0	0	0.05278	0.06820
$\nu_2$	-1.81712	-0.33349	0.01439	0.26760	2.02267	8.04999
$\delta \nu_2$	0.10000	0.02220	0.00099	0.01859	0.04989	0.11795
$\nu_3$	13.000	1.9280	-0.13021	-1.5000	-9.7304	-53.865
$\delta \nu_3$	0.18571	0.04000	0.00298	0.03571	0.50498	0.13402

### C. Restriction on applying hypervirial relations

As noticed, there are some cases in which the expectation value  $\langle R_{twf} | [G, H] | R_{twf} \rangle$  vanishes accidentally. We list following possible cases:

- (i) TWF is an eigenstate of  $G$ ,
- (ii) TWF is an eigenstate of the commutator  $[G, H]$  with eigenvalue 0,
- (iii)  $G|R_{twf}\rangle$  is orthogonal to  $H|R_{twf}\rangle$ ,
- (iv)  $[G, H]|R_{twf}\rangle$  is orthogonal to  $|R_{twf}\rangle$ .

Evidently, in these cases the corresponding hypervirial relation cannot be used as a criterion. Table 1 indicates that we just confront this case for the 1S state in the linear potential. The optimal TWF (B1) gives  $\nu_1 \equiv 0$  and the result is independent of the value of  $b$ .

In fact, since we choose  $G_1 = rp_r$  as the first order hypervirial operator which is just the generator of the dilation  $W$  and has no Hilbert-space eigenvector [3], with  $N=1$  and Eq.(20), we have

$$[rp_r, H] = 3r - 2H. \quad (32)$$

One can straightforwardly prove that for the optimal TWF of the ground state,  $R_{twf}(r)$  in the form of Eq. (B1),  $[rD, H]|R_{twf}\rangle$  is orthogonal to the state  $|R_{twf}\rangle$ . Thus, this is the case (iv) and the 1-st order hypervirial relation cannot be used to judge the quality of the concerned TWF. Definitely, in this case, we can use  $\nu_2$  which is not equal to zero and can sensitively judge the accuracy of the concerned TWF. To our knowledge, the authors of most literatures only discussed the possibility for the case where the hypervirial relation fails to testify the given trial function, but seldom gave concrete examples. The form of TWF (B1) presented by us is a convincing illustration.

We find that at this point we can give stronger arguments and generalize it to extensive cases. Epstein and Hirschfelder have proved a well-known lemma [10] which states that if a variational trial function  $\psi$  obeys

$$\frac{\partial\psi}{\partial a} = iW\psi \quad (33)$$

where  $a$  is the variational parameter and  $W$  is a Hermitian operator, then the optimal  $\psi$  satisfies the hypervirial theorem for the Hermitian operator  $W$ , i.e.

$$\langle\psi|[W, H]|\psi\rangle = 0.$$

The authors of ref. [11] generalized the lemma and claimed that if Eq. (33) is replaced by

$$\frac{\partial\psi}{\partial a} = BiW\psi + iC\psi, \quad (34)$$

the lemma is still correct. In Eq.(34)  $B$  and  $C$  are the functions of  $a$ ,  $B$  is real and  $W$  is Hermitian. Evidently, Eq.(33) is a special case of Eq.(34) with  $B = 1$  and  $C = 0$ . This lemma and its generalized form have extensively been used to select approximate TWF's and to discuss the spectroscopy of molecule and atom.

Later, as a sample of the application of the generalized lemma, we will stay in the linear potential case, unless it is specially specified.

With this generalized lemma, we can deduce some very useful consequences.

(a) For the  $1S$  state, when TWF is in the form (B1), we have

$$\frac{\partial R_{twf}(r)}{\partial a} = (\frac{3}{2ab} - r^b)R_{twf}(r). \quad (35)$$

As aforementioned, taking

$$W = \frac{1}{2}(rp_r + p_r r) = -i(r\frac{d}{dr} + \frac{3}{2}) \quad (36)$$

as the hypervirial operator, we get

$$iWR_{twf}(r) = (\frac{3}{2} - abr^b)R_{twf}(r). \quad (37)$$

Comparing (37) with (35), we can obtain

$$\frac{\partial R_{twf}(r)}{\partial a} = \frac{1}{ab}iWR_{twf}(r), \quad (38)$$

which corresponds to  $B = -\frac{1}{ab}$  and  $C = 0$  in Eq.(34). When the variational parameter  $a$  takes its optimal value, we must have  $\nu_1 = 0$ , which is independent of the value  $b$ . This means that the optimal TWF (B1) for the  $1S$  state satisfies the general virial theorem although it is not the exact wave function. If the employed TWF is of this kind, we at least have to use the second order hypervirial relation  $\nu_2$ .

(b) In fact, (a) can be generalized to the other cases, because the result is independent of the concrete form of the central potential  $V(r)$ . As long as we take Eq. (B1) as TWF for the

1S state in any central potential case, the general virial theorem must be satisfied, namely  $\nu_1 = 0$ . The general virial theorem cannot be taken as a criterion to judge the quality of TWF. Then, we have to use the deviations from 2-nd and 3-rd order hypervirial relations  $\nu_2$  and  $\nu_3$  as the criteria.

To investigate the applications of the above consequence, we evaluate  $\nu_i$ 's with the frequently used potential forms including (i) the Coulomb potential, (ii) the Cornell potential  $V(r) = -\frac{1}{r} + r$ , (iii) the Martin potential  $V(r) = r^{0.1}$ , (iv) the logarithmic potential  $V(r) = \log(r)$  and (v) the three dimensional isotropic oscillator potential  $V(r) = r^2$ , respectively. The expressions of  $\nu_i$  and  $\delta\nu_i$  ( $i=1,2,3$ ) obtained from the general formula and the corresponding numerical results for these potentials are shown in Table 2.

It can be seen from the table that for the cases , (ii) , (iii) and (iv), when  $b = \frac{3}{2}$ , one obtains the best TWF. On the other hand, in the case (i) (or (v)), the closer to 1 (or 2) the value of  $b$  is, the smaller the corresponding  $\delta\nu_2$  and  $\delta\nu_3$  are. Eventually, when  $b = 1$  (or 2), the TWF is just the exact solution for the corresponding potential and all  $\nu_i$  and  $\delta\nu_i$  go to zero. Obviously, one can use  $\delta\nu_2$  and  $\delta\nu_3$  as the criteria to judge whether TWF is accurate enough.

Table 2

Variational results with the single-parameter TWF (B1) in some central potentials cases mentioned in the text.

$b$	1	$\frac{3}{2}$	$\frac{7}{4}$	2
Coulomb potential $V(r) = -\frac{1}{r}$				
$a_0$	0.50000	0.19159	0.11770	0.07074
$E$	-0.25000	-0.23555	-0.22400	-0.21221
$\nu_1 \equiv -\langle 1/r \rangle - 2E$	0	0	0	0
$\nu_2 \equiv -3 - 4E\langle r \rangle$	0	-0.31289	-0.39463	-0.45352
$\nu_3 \equiv -5\langle r \rangle - 6E\langle r^2 \rangle - 3$	0	-3.1523	-3.9158	-4.5000
$\delta\nu_2 \equiv \frac{ \nu_2 }{3}$	0	0.10439	0.13154	0.15117
$\delta\nu_3 \equiv \frac{ \nu_3 }{5\langle r \rangle}$	0	0.01543	0.01931	0.02122
Cornell potential $V(r) = -1/r + r$				
$a_0$	1.10939	0.63544	0.49016	0.37969
$E$	1.47345	1.39969	1.41824	1.45064
$\nu_1 \equiv 3\langle r \rangle - \langle \frac{1}{r} \rangle - 2E$	0	0	0	0
$\nu_2 \equiv 5\langle r^2 \rangle - 4E\langle r \rangle - 3$	1.21878	-0.08892	-0.40439	-0.63714
$\nu_3 \equiv 7\langle r^3 \rangle - 6E\langle r^2 \rangle - 5\langle r \rangle - 3$	7.1409	-0.35635	-1.8015	-2.7949
$\delta\nu_2 \equiv \frac{ \nu_2 }{5\langle r^2 \rangle}$	0.10000	0.00881	0.04094	0.06514
$\delta\nu_3 \equiv \frac{ \nu_3 }{7\langle r^3 \rangle}$	0.18571	0.01370	0.07375	0.11708
Martin potential $V(r) = r^{0.1}$				
$a_0$	0.24300	0.06770	0.03641	0.01965
$E$	1.24007	1.23576	1.23654	1.23811
$\nu_1 \equiv 2.1\langle r^{0.1} \rangle - 2E$	0	0	0	0
$\nu_2 \equiv 4.1\langle r^{1.1} \rangle - 4E\langle r \rangle$	0.26731	-0.01636	-0.08947	-0.14441
$\nu_3 \equiv 6.1\langle r^3 \rangle - 6E\langle r^2 \rangle - 3$	6.6550	-0.41743	-1.8517	-2.8500
$\delta\nu_2 \equiv \frac{ \nu_2 }{4.1\langle r^{1.1} \rangle}$	0.00865	0.00058	0.00320	0.00515
$\delta\nu_3 \equiv \frac{ \nu_3 }{6.1\langle r^3 \rangle}$	0.01717	0.00140	0.00645	0.01005
Logarithmic potential $V(r) = \log(r)$				
$a_0$	0.70711	0.33693	0.23663	0.16667
$E$	1.07521	1.0450	1.05310	1.06755
$\nu_1 \equiv 2\langle \log(r) \rangle + 1 - 2E$	0	0	0	0
$\nu_2 \equiv 4\langle r \log(r) \rangle - (4E - 1)\langle r \rangle$	0.70711	-0.08362	-0.28942	-0.44455
$\nu_3 \equiv 6\langle r^2 \log r \rangle - (6E - 1)\langle r^2 \rangle - 3$	6.0000	-0.67223	-2.0412	-3.0000
$\delta\nu_2 \equiv \frac{ \nu_2 }{4\langle r \log(r) \rangle}$	0.09162	0.01362	0.04854	0.07474
$\delta\nu_3 \equiv \frac{ \nu_3 }{6\langle r^2 \log r \rangle}$	0.14374	0.02480	0.08129	0.12334
3-D isotropic oscillator potential $V(r) = r^2$				
$a_0$	1.3161	0.78082	0.52127	0.50000
$E$	3.4641	3.0667	3.0136	3.0000
$\nu_1 \equiv \langle r^2 \rangle - E/2$	0	0	0	0
$\nu_2 \equiv 6\langle r^3 \rangle - 4E\langle r \rangle$	3.9482	1.0499	0.43243	0
$\nu_3 \equiv 8\langle r^4 \rangle - 6E\langle r^2 \rangle - 3$	21.000	4.63819	1.81366	0
$\delta\nu_2 \equiv \frac{ \nu_2 }{6\langle r^3 \rangle}$	0.37992	0.11412	0.04783	0
$\delta\nu_3 \equiv \frac{ \nu_3 }{8\langle r^4 \rangle}$	0.35000	0.12937	0.05657	0

### D. Application to the 1P case

Now, let us turn to the 1P state. The wavefunction for the 1P state is  $R_{1p}(r)Y_{1m}(\theta, \phi)$ . For the linear potential case, the differential equation for  $R_{1p}(r)$  reads

$$\left[-\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \frac{2}{r^2} + r\right]R_{1p}(r) = E R_{1p}(r). \quad (39)$$

There is no analytical solution for  $R_{1p}(r)$ . Although one can solve it numerically, if we use the variational method to find an optimal TWF for the 1P state, we would not have a convenient exact solutions like Airy function for the S state to compare with. In this case, only the hypervirial relations can serve as a powerful measure to judge the quality of TWF.

Now, we write the optimal TWF in a more general form

$$R_{twf}^{(n)}(r) = N_n r^n e^{-ar^b} \quad (n = 1), \quad (40)$$

with the normalization constant  $N_n$  being

$$N_n = (2a)^{\frac{3+2n}{2b}} \sqrt{\frac{b}{\Gamma(\frac{3+2n}{b})}} \quad (n = 1). \quad (41)$$

It is very easy to prove that this TWF also satisfies the general virial theorem, namely  $\nu_1 = 0$ . Because we have

$$\frac{\partial R_{twf}^{(n)}(r)}{\partial a} = \left(\frac{3+2n}{2ab} - r^b\right) R_{twf}^{(n)}(r) \quad (42)$$

and

$$iW R_{twf}^{(n)}(r) = \left(\frac{3}{2} + n - abr^b\right) R_{twf}^{(n)}(r), \quad (43)$$

comparing (42) with (43), we can immediately reach Eq.(38). Actually,  $R_{twf}(r)$  is a special case of TWF  $R_{twf}^{(n)}(r)$  with  $n = 0$ .

Taking  $n = 1$ , one has the 1P state TWF

$$R_{twf}^{(1)}(r) = N_1 r e^{-ar^b}. \quad (44)$$

We can fix the optimal values of the variational parameter  $a$  and the energy  $E$  for  $b = 1, \frac{3}{2}, \frac{7}{4}$  and 2, respectively, according to the normal procedure, and the results are shown in Table 3. The analytical expressions and their numerical results of the deviation from the first and second hypervirial relations  $\nu_1, \nu_2$  and  $\delta\nu_2$  are also shown in the table.

It is easy to see from Table 3 that

(a)  $\nu_1$  is indeed zero, which is independent of the value of  $b$ . This is consistent with our general discussion on the TWF  $R_{twf}^{(n)}(r)$ ;

(b) The optimal value of  $a$  is different from the one for 1S state, and  $\delta\nu_2$  can sensitively be used to select the best TWF. The result is  $b = \frac{7}{4}$  again. This conclusion is consistent with that achieved for the 1S state.

Table 3

Variational results with the single-parameter TWF Eq.(44) for the 1P state in the linear potential case.

$b$	1	$\frac{3}{2}$	$\frac{7}{4}$	2
$a_0$	1.07722	0.47141	0.32323	0.22452
E	3.48119	3.36927	3.36135	3.36778
$\nu_1 \equiv 3\langle r \rangle - 2E$	0	0	0	0
$\nu_2 \equiv 5\langle r \rangle + 4\langle \frac{1}{r} \rangle - 4E\langle r \rangle$	2.15443	0.45059	-0.02146	-0.39152
$\delta\nu_2 \equiv \frac{ \nu_2 }{5\langle r^2 \rangle + 4\langle \frac{1}{r} \rangle}$	0.06250	0.01467	0.00071	0.01311

Instead, if we still employ a TWF in the form of

$$R_{1p}(r) = c_0 r e^{-a_0 r^{\frac{7}{4}}}, \quad (45)$$

where  $a_0$  is taken to be the optimal value for the  $1S$  state and  $c_0$  is determined by the normalization condition. Then, there is no free parameter. Calculating  $\langle H \rangle$ , one can straightforwardly obtain the energy

$$E = 3.6788.$$

The corresponding deviations from the first and second order hypervirial relations are

$$\nu_1 = -0.1003 \quad \delta\nu_1 = 0.04676,$$

and

$$\nu_2 = -1.0472 \quad \delta\nu_2 = 0.03760,$$

respectively. This is because that the Hamiltonian for the  $1P$  state is different from that for the  $1S$  state, so that the adopted  $a_0$  is not the optimal value for the  $1P$  state, and the  $R_{1p}(r)$  given by (45) does not satisfy the general virial theorem, namely  $\nu_1$  is not equal to zero.

In comparison with the values of  $\nu_2$  and  $\delta\nu_2$  in Table 3 for  $b = \frac{7}{4}$ , one can conclude that the TWF chosen in such a way is not an appropriate one.

Now, we add one more variational parameter in and take TWF in the form of

$$R_{1p}(r) = (c_0 + c_1 r) r e^{-a_0 r^{\frac{7}{4}}}, \quad (46)$$

where  $a_0$  still takes the value in Eq.(45),  $c_0$  is determined by the normalization condition and  $c_1$  is a new variational parameter. By using variational method, we have

$$E = 3.36202$$

and

$$\nu_1 = -0.01177 \quad \delta\nu_1 = 0.00528,$$

$$\nu_2 = -0.25348 \quad \delta\nu_2 = 0.008526.$$

Evidently, the accuracy of TWF is much more improved.

### E. The other possible choice for the hypervirial operator

One may choose different hypervirial operators  $G$  instead of what we employed above. Here, we give another example where the new hypervirial operator  $G'$  is in the form of

$$G' = f(r)p_r^2.$$

With the Hamiltonian

$$H = p_r^2 + V_{eff}(r)$$

where

$$V_{eff}(r) = \frac{l(l+1)}{r^2} + V(r),$$

we have the commutator

$$[H, G'] = f(r) \frac{d^2 V_{eff}(r)}{dr^2} + 2if(r) \frac{dV_{eff}(r)}{dr} p_r - \frac{d^2 f(r)}{dr^2} p_r^2 - 2i \frac{df(r)}{dr} p_r^3. \quad (47)$$

Let us set  $l = 0$  and  $V(r) = r$  for demonstration. Taking  $f(r) = r$ , we obtain a new first order hypervirial relation

$$\langle -irp_r \rangle = \langle -ip_r^3 \rangle. \quad (48)$$

Similar to above operation, we define

$$\nu'_1 \equiv \langle -ip_r^3 \rangle - \langle -irp_r \rangle \quad (49)$$

and

$$\delta\nu'_1 \equiv \frac{|\nu'_1|}{\langle -ip_r^3 \rangle} \quad (50)$$

as a criterion to judge the quality of a TWF. However, considering

$$p_r^2 = H - r,$$

$$p_r r + r p_r = -i + 2r p_r$$

and Eq.(48), it is possible to give an alternative expression for the criterion, which reads

$$\nu''_1 \equiv E \langle -ip_r \rangle + 1 - 2 \langle -irp_r \rangle. \quad (51)$$

Because for any eigenstate  $|R_{eig}\rangle$  of the Hamiltonian  $H$  we have

$$H|R_{eig}\rangle = E|R_{eig}\rangle, \quad (52)$$

$\nu'_1$  is identical to  $\nu''_1$  for the exact solution. For an approximate solution, these two expressions would give different results. However, it is not difficult to prove that for any function  $R(r) = u(r)/r$  which satisfies the normalization condition (A3) and the boundary condition (A4), we surely have

$$\langle -ip_r \rangle = 0 \quad (53)$$



and

$$\langle -irp_r \rangle = \frac{1}{2}. \quad (54)$$

Consequently,  $\nu_1''$  vanishes trivially and cannot be used as a criterion. In general,  $\nu_1'$  is not zero. Therefore,  $\nu_1'$  and  $\delta\nu_1'$  can be applied to judge the quality of a TWF. We list the numerical result for the  $1S$  state with the TWF parameters used in(B1) in Table 4.

Table 4

Variational results with the single-parameter TWF (B1) for the  $1S$  state in the linear potential case. The employed hypervirial operator is  $G'$ .

$b$	1	$\frac{3}{2}$	$\frac{7}{4}$	2
$\nu_1'$	1	0.16667	0.018228	-0.07559
$\delta\nu_1'$	0.6667	0.25000	0.03517	0.17810

It is easy to see from Table 4 that  $\delta\nu_1'$  can indeed be used as a criterion to judge the quality of the TWF and gives a consistent result with those in Table 1, but it is less sensitive than  $\delta\nu_2$  presented in Table 1.

#### IV. CONCLUSION AND DISCUSSION

There are a variety of approximation methods which can be employed to solve the non-relativistic Schrödinger equation where exact analytical solutions cannot be obtained. The variational method is one of the most frequently adopted approaches because of its apparent advantages. As well known, the obtained eigenenergies and wavefunctions are closely related to the form of the variational trial wavefunction (TWF) and the number of the variational parameters. What we concern is how close to the real values the achieved results can be. This is a crucial problem which should tell us the reliability of the results. In other words, we need a proper way to judge the quality of the TWF, especially the single-parameter TWF, because of its simplicity.

To answer this question, we can set some criteria which determine the quality of the adopted TWF. In this work, we have carefully studied several calculable quantities for this purpose. Some of them were suggested in literatures and the rest of them are newly introduced by us. To obtain the idea of the criterion for judging the quality of TWF, we use the simple potential form  $V(r) = r$ , which has exact solutions for  $nS$  states, as an example. The numerical results indicate that all the criteria are consistent, namely, if one of them shows a sufficiently smaller deviation of the obtained result from the exact solution, the others confirm the conclusion. However, except the hypervirial relations, evaluating the quantities which stand for the criteria of the quality of TWF needs the exact solutions of the Schrödinger equation. Apparently, such solutions are generally not available. Only can the deviations from the hypervirial relations serve as a practical and powerful criterion for the

quality of TWF. Furthermore, in our special case with  $V(r) = r$ , we can deduce a conclusion that the hypervirial relations can be a good criterion and is supported by the other criteria gained in the special case where the exact solutions for  $nS$  states are available. This is also valid for various potential forms. To consolidate our confidence, we have studied the  $1P$  state with  $V(r) = r$ , where no exact solution exists. The results are qualitatively and quantitatively consistent with what we expected.

Moreover, we use  $G = r^N p_r$  as the hypervirial operator which is of obvious physical significance. It should be specially noticed that in some special or accidental cases, the first (maybe the first a few) hypervirial relations precisely hold. However, it is not due to the correctness of TWF, but the TWF's fall in the special categories which are specified in Sec.III(D). In these cases, the first a few hypervirial relations cannot be used as criteria for the quality of TWF, instead one needs to invoke higher orders hypervirial relations or use other hypervirial operator, for example,  $G'$  in Sec.III(E). Thus, when one applies the hypervirial relations as criteria for the quality of TWF, he has to study the form of the adopted TWF to see if it falls into the categories listed in Sec.III(D).

Our conclusion affirms that the hypervirial relations hold precisely for the real eigenstates, but approximately for TWF. They can be used to determine the quality of the adopted TWF. The deviation of the hypervirial relations from equality can serve as the most practical and powerful criterion for choosing an appropriate TWF in any potential cases.

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## APPENDIX A: THE ANALYTICAL SOLUTION OF THE SCHÖDINGER EQUATION FOR $S$ -STATES IN THE LINEAR POTENTIAL CASE

In the framework of the non-relativistic potential model, with a central potential  $V(\vec{r}) = V(r)$ , the eigenstate energy  $E$  and the corresponding radial wave function  $R(r)$  can be obtained by solving the Schrödinger equation

$$H R(r) \equiv \left[ \frac{p_r^2}{2\mu} + \frac{l(l+1)}{2\mu r^2} + V(r) \right] R(r) = E R(r), \quad (\text{A1})$$

where  $H$  is the Hamiltonian,  $\mu$  the reduced mass,  $p_r$  the radial momentum operator and  $l$  the quantum number of the angular momentum. The radial wave function  $R(r)$  satisfies the normalization condition:

$$\int_0^\infty R^2(r) r^2 dr = 1. \quad (\text{A2})$$

Taking the linear potential  $V(r) = r/r_0$  normalized as  $r_0 = 1/\text{GeV}^2$  (so we ignore  $r_0$  in all later expressions),  $2\mu = 1 \text{ GeV}$  and the reduced radial wave function  $u(r) = r R(r)$  which satisfies the normalization condition

$$\int_0^\infty u^2(r) dr = 1, \quad (\text{A3})$$

and the boundary condition

$$u(0) = 0 \quad \text{and} \quad u(\infty) = 0. \quad (\text{A4})$$

The equation for the  $S$  state has a simple form:

$$\left(-\frac{d^2}{dr^2} + r\right)u(r) = Eu(r). \quad (\text{A5})$$

Rewriting the equation as

$$\left(\frac{d^2}{dr^2} + (E - r)\right)u(r) = 0, \quad (\text{A6})$$

and comparing it with the Airy equation [12]

$$\left(\frac{d^2}{dz^2} - z\right)W(z) = 0, \quad (\text{A7})$$

one easily obtains

$$u_{nS}(r) = N_n \text{Ai}(r - E_n), \quad (n = 1, 2, 3, \dots \text{ and } r \geq 0) \quad (\text{A8})$$

where  $\text{Ai}(z)$  is the Airy function,  $N_n$  the normalization constant and  $E_n$  the eigenenergy of the  $nS$  state in the linear potential case, which is just the value of the negative  $n$ -th node of the Airy function  $\text{Ai}(z)$ . The numerical values of  $E_n$  are  $E_1 = 2.33810 \dots$ ,  $E_2 = 4.08794 \dots$ ,  $E_3 = 5.52055 \dots$  etc., respectively.

## APPENDIX B: THE VARIATIONAL SOLUTION FOR THE $S$ -STATES IN THE LINEAR POTENTIAL CASE

For the ground state, i.e. the  $1S$  state, in the linear potential case with  $2\mu = 1\text{GeV}$ , the nomarlized trial wave function (TWF) with a single variational parameter is taken to be

$$R_{twf}(r) = N e^{-a r^b}, \quad (\text{B1})$$

with the normalization constant

$$N = \left[ \frac{b (2a)^{\frac{3}{b}}}{4\pi\Gamma(\frac{3}{b})} \right]^{\frac{1}{2}}. \quad (\text{B2})$$

In above equations,  $a$  denotes the variational parameter and  $b$  represents the model parameter which specifies the type of the TWF. If one considers the linear potential only, the Hamiltonian for the  $nS$  state can be written as

$$H = -\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + r, \quad (\text{B3})$$

Solving the Schödinger equation in terms of the TWF Eq.(B1), one obtains the analytical results for  $a_0$  and  $E$ . The optimal value of  $a$  is

$$a_0 = \frac{1}{2} \left( \frac{2\Gamma(\frac{4}{b})}{(1+b)\Gamma(\frac{1}{b})} \right)^{\frac{b}{3}}, \quad (\text{B4})$$

and the corresponding minimum value of the energy reads

$$E_{min} = \frac{3}{2\Gamma(\frac{3}{b})} \left( \frac{(1+b)\Gamma(\frac{1}{b})\Gamma^2(\frac{4}{b})}{2} \right)^{\frac{1}{3}}. \quad (\text{B5})$$

Because the behavior of the linear potential lies between the Coulomb potential and the harmonic oscillator potential, we select four kinds of TWF with  $b = 1$  ( "hydrogen-like" wave function ),  $b = \frac{3}{2}$ ,  $b = \frac{7}{4}$  and  $b = 2$  ( Gaussian wave function ), respectively. The resultant  $a_0$  and  $E_{min}$  for various values of  $b$  are shown in Table 1. It is clear that when  $b = 7/4$ , one reaches the most accurate solution.

Taking  $b = 7/4$ , one can construct a TWF for the  $2S$  state. It reads

$$R_{twf}^{2S}(r) = (c_0 + c_1 r + c_2 r^2) e^{-a_0 r^{\frac{7}{4}}}, \quad (\text{B6})$$

where  $a_0 = 0.348957$ , which is the optimal value determined for the  $1S$  state,  $c_0$  can be given by the normalization condition,  $c_1$  should be determined by the orthogonal condition to the  $1S$  state and  $c_2$  is the unique variational parameter which can be obtained by minimizing the corresponding average value of the Hamiltonian  $H$ ,  $\langle R_{twf}^{2S} | H | R_{twf}^{2S} \rangle$ .

Similarly, for the  $3S$  state, we can take TWF as

$$R_{twf}^{3S}(r) = (c_0 + c_1 r + c_2 r^2 + c_3 r^3) e^{-a_0 r^{\frac{7}{4}}}. \quad (\text{B7})$$

The numerical values for the  $2S$  and  $3S$  states are also shown in Table 1.

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